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Detonation Shock Dynamics (DSD) Calibration for LX-17

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1. INTRODUCTION

The goal of this report is to summarize the results of a DSD calibration for the explosive LX-17. Considering that LX-17 is very similar to PBX 9502 (LX-17 is 92.5% TATB with 7.5% Kel-F 800 binder, while PBX 9502 is 95% TATB with 5% Kel-F 800 binder), we proceed with the analysis assuming many of the DSD constants are the same. We only change the parameters D_{CJ}, B and $\overline{C}_6$ ($\overline{C}_6$ controls the how D_{CJ} changes with pressing density). The parameters D_{CJ} and $\overline{C}_6$ were given by Josh Coe and Sam Shaw's EOS. So, only B was optimized in fitting all the calibration data. This report first discusses some general DSD background, followed by a presentation of the available dataset to perform the calibration, and finally gives the results of the calibration and draws some conclusions.

A set of parameters for Detonation Shock Dynamics (DSD) normal shock velocity, D_n, versus curvature, κ, propagation law shall be calibrated. The general form used in codes of the $D_n(\kappa)$ law has as parameters (D_{CJ}, A, B, C_1, C_2, C_3, C_4, C_5, e_1, e_2, e_3, e_4, e_5) [1]:

$$\frac{D_n}{D_{CJ}} = 1 + A\left(\left(C_1 - \kappa\right)^{e_1} - C_1^{e_1}\right) - B\kappa\left(\frac{1 + C_2\kappa^{e_2} + C_3\kappa^{e_3}}{1 + C_4\kappa^{e_4} + C_5\kappa^{e_5}}\right). \tag{1}$$

In addition to the above parameters, the maximum allowable curvature, κ_{max}, and the sonic edge angle, ω_s, are required to fully specify the DSD parameter list. Note that the RHS and LHS, given above, are dimensionless. Also, all velocity scales are contained on the left, while the length scales are on the right. We take the following $D_n(\kappa)$, which is simple reconfiguration of the original one above (the "A" term has been removed, because it was not needed to adequately fit the experimental data for PBX 9502):

$$\frac{D_n}{D_{CJ}} = 1 - B\kappa\left(\frac{1 + \overline{C}_2\left(B\kappa\right)^{e_2} + \overline{C}_3\left(B\kappa\right)^{e_3}}{1 + \overline{C}_4\left(B\kappa\right)^{e_4} + \overline{C}_5\left(B\kappa\right)^{e_5}}\right). \tag{2}$$

Note that B has been brought into the κ terms in the ratio, so as to define new dimensionless parameters $\overline{C}_2, \overline{C}_3, \overline{C}_4, \overline{C}_5$, with $C_2 = \overline{C}_2 B^{e_2}$, etc. Furthermore, we assume the length scale, B, to vary according to (as was done previously for the Aug 2011 PBX 9502 DSD calibration, [2]):

$$B = B_{LX-17}\left(\left(\frac{\rho_0}{\rho_{0_{\text{nominal}}}}\right)^{\overline{C}_7} - \overline{C}_9\left(\frac{T_0}{T_{0_{\text{nominal}}}} - 1\right) + \overline{C}_{10}\left(\frac{T_0}{T_{0_{\text{nominal}}}} - 1\right)^2\right), \tag{3}$$

and D_{CJ} to vary according to:

$$D_{CJ} = D_{CJ_{\text{nominal}}}\left(1 + \overline{C}_6\left(\frac{\rho_0}{\rho_{0_{\text{nominal}}}} - 1\right) - \overline{C}_8\left(\frac{T_0}{T_{0_{\text{nominal}}}} - 1\right)\right) \tag{4}$$

where the nominal temperature and density (nominal density from Josh Coe and Sam Shaw) are taken as:

$$T_{0_{\text{nominal}}} = 298.15 \text{ K}$$
$$\rho_{0_{\text{nominal}}} = 1.903 \text{ g/cc}$$

Note that D_{CJ} and B were assumed to vary only with temperature and pressed density. Furthermore, the dimensionless parameters $\overline{C}_2, \overline{C}_3, \overline{C}_4, \overline{C}_5, \overline{C}_7, \overline{C}_8, \overline{C}_9, \overline{C}_{10}$ are assumed to be intrinsic characteristics of PBX 9502 and LX-17, and are not assumed to vary with temperature and pressed density. The $\overline{C}_6$ parameter is chosen to yield $dD_{CJ}/d\rho_0$ = 3.495 (m/s)/(mg/cm^3), from Josh Coe and Sam Shaw, and thus must be $\overline{C}_6 = 0.85930$. This leaves us with only determining B_{LX-17}.

2. LX-17 RATESTICK DATA

The calibration of the B_{LX-17} parameter utilized rate stick data from the LLNL Explosives Reference Guide [3]. These experimental results are also available in the open literature [4] [5]. Table 1 summarizes this diameter effect data (as it appeared in [3] in November, 2011).

LLNL Shot #	Radius mm	Pressed Density g/cm^3	Detonation Velocity mm/μs	Measured Std. Dev. mm/μs
617	12.718	1.887	7.522	0.013
618	12.718	1.893	7.509	0.015
624	12.660	1.902	7.543	0.027
765	9.486	1.903	7.485	0.009
764	7.794	1.905	7.443	0.038
732	7.790	1.915	7.465	0.026
756	7.283	1.910	7.478	0.046
766	6.355	1.908	7.499	0.030
733	6.330	1.920	7.473	0.051
763	5.554	1.902	7.384	0.017
754	5.553	1.910	7.412	0.056
744	6.330	1.910	7.437	0.037

Table 1. Rate stick experimental data used in current calibration, from [3].

3. BEST FIT (CALIBRATION) TO LX-17 RATESTICK DATA

One can calibrate the $D_n(\kappa)$ parameters to yield a good comparison for both the shock shapes and phase velocities (i.e. "diameter effect"). Here the intent is to minimize a merit function, E, which is a combination of differences between theory and experimental phase speeds (diameter effect) and differences between theory and experimental shock shapes:

$$E = w\left(\frac{E_{DE}}{E_{DEbest}}\right)^2 + (1-w)\left(\frac{E_{SS}}{E_{SSbest}}\right)^2 \tag{5}$$

where E_{DE} is the error in diameter effect (note that each difference is scaled by the measured standard deviation for that experiment, since those standard deviations were both large in magnitude and more importantly varied significantly across shots – effectively experiments with large uncertainty are weighted less than those with small uncertainty) :

$$E_{DE} = \frac{1}{N_r}\left(\sum_1^{N_r}\left(\frac{D_{0data} - D_{0DSD}}{MeasStdDev}\right)^2\right)^{1/2} \tag{6}$$

where N_r is the number of records and D_{0data} and D_{0DSD} are the experimentally observed and DSD calculated phase speeds respectively for each record. E_{SS} is the error in shock shape:

$$E_{SS} = \frac{1}{N_r}\left(\sum_1^{N_r}\frac{1}{N_{data}}\sum_1^{N_{data}}\left(z_{data} - z_{DSD}\right)^2\right)^{\frac{1}{2}} \tag{7}$$

where z_{data} and z_{DSD} are the experimental and DSD calculated shock displacements respectively. N_{data} is the number of experimental points recorded along the shock location.

Here, E_{DEbest} is the lowest error found in diameter effect without regard to the resulting errors in shock shapes. E_{SSbest} is the lowest error found in shock shape without regard to errors in diameter effect. The above formulation, Eqn (5), is a convenient way to combine phase speed and shock shape in a dimensionally consistent fashion. The weight, w, is used to balance between diameter effect and shock shape. In this study w=2/3 was used, but is obviously not unique (nor is the metric unique). The parameter w=2/3 was also used in the PBX 9502 fitting.

As stated earlier, not all the parameters in the $D_n(\kappa)$ are needed to fit this data set adequately. In general, we take e_2=e_4=1 and e_3=e_5=2. Furthermore, choosing A=0 still gave plenty of flexibility to fit the data. Again, only $B_{LX\text{-}17}$ is being fit. The parameters are given in Table 2 below. Lastly, as was the case for PBX 9502, I chose to take κ_{max} =3.5 mm^{-1}, to allow $D_n(\kappa_{max}) < D_0 \sin(\omega_s)$, which is needed to allow for correct implementation of the boundary condition angles for detonations in rate sticks with phase speeds of D_0. Note that ω_s corresponds to a shock deflection angle of ~35°, the same as used for PBX 9502.

$D_{CJ\mathrm{nominal}}$	7.740 mm/μs
κ_{max}	3.5 mm^{-1}
$B_{\mathrm{LX\text{-}17}}$	3.9764 mm
$\overline{C}_2$	4.8707
$\overline{C}_3$	2.7768
$\overline{C}_4$	32.115
$\overline{C}_5$	78.183
$\overline{C}_6$	0.85930
$\overline{C}_7$	30.819
$\overline{C}_8$	0.027099
$\overline{C}_9$	1.8654
$\overline{C}_{10}$	2.0377
ω_s	0.9599

Table 2. LX-17 optimal DSD parameters. Only the red entries differ from [2].

This set of parameters yields a $D_n(\kappa)$ curve (at nominal density of 1.903 g/cm^3) given in Figure 3. Also shown in Fig. 3 are two PBX 9502 $D_n(\kappa)$ curves for comparison. Note that at κ=0, D_n for PBX 9502 is 7.800 mm/μs, while for LX-17 it is 7.740 mm/μs. At very high curvature, the LX-17 curve crosses the PBX 9502 HOL88H891-008 lot, but does not cross the PBX 9502 LANL79-04 lot. This is due to the fact that:

$$B_{\mathrm{LANL79\text{-}04}} < B_{\mathrm{LX\text{-}17}} < B_{\mathrm{HOL88H891\text{-}008}}. \qquad (8)$$

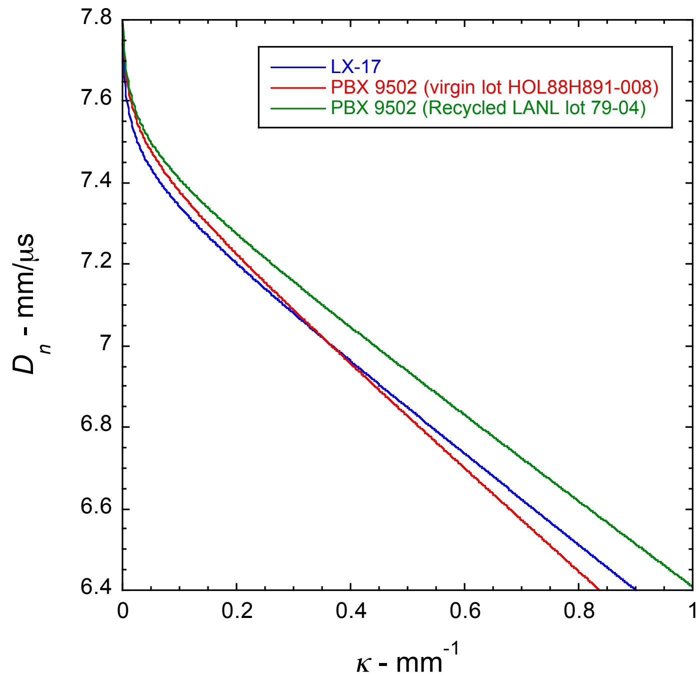

Figure 3. LX-17 $D_n(\kappa)$ calibration at nominal density and temperature. Also shown, for comparison, are 2 different PBX 9502 $D_n(\kappa)$ curves.

The resulting LX-17 diameter effect curve is given in Figure 4 (corrected to nominal density). The shock shape residuals, comparing DSD with experimental data, is presented in Figure 5.

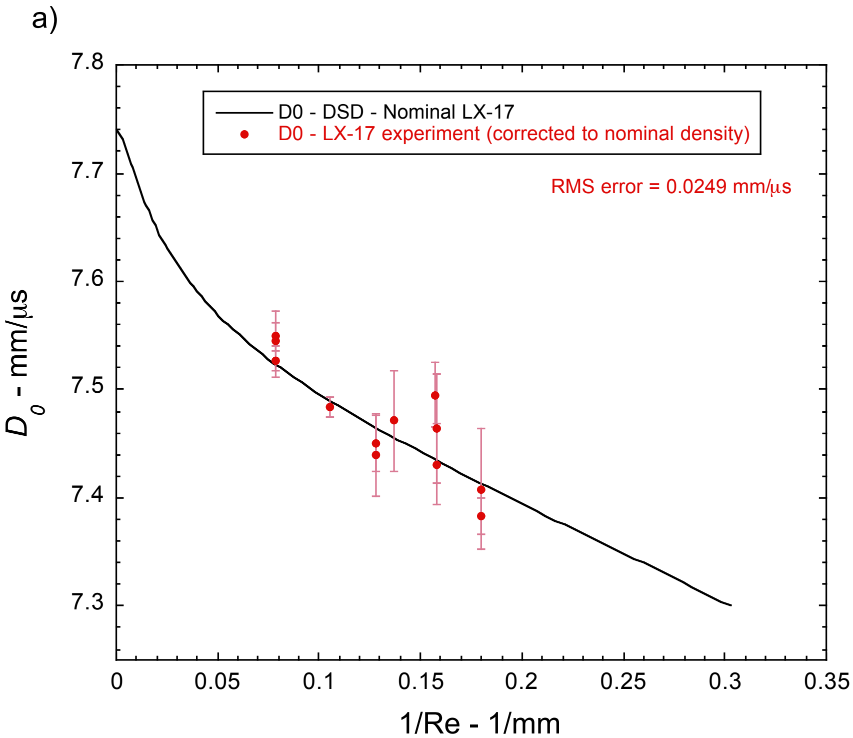

Figure 4. a) Calibrated LX-17 DSD diameter effect at nominal density, experimental data (corrected to nominal density) and experimental measured standard deviations.

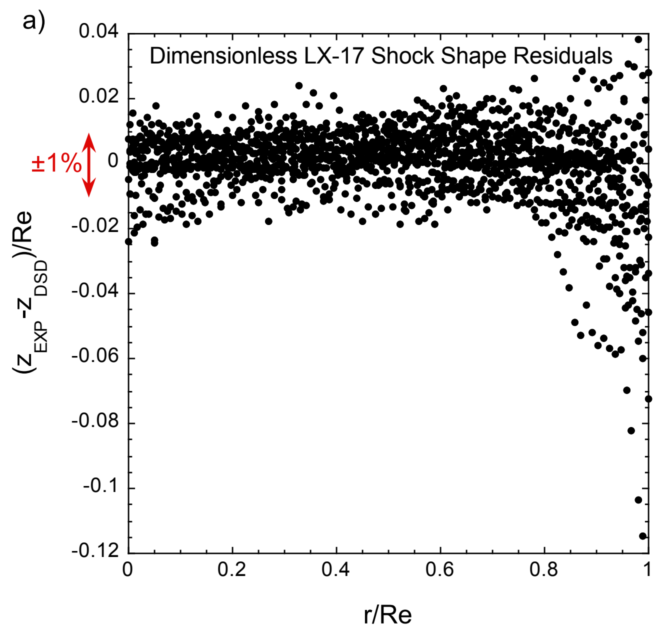

Figure 5. Difference in experimental and DSD calculated shock shapes scaled by radius of charge for both axes. a) LX-17, all 11 experimental comparisons shown.

5. CONCLUSIONS

A DSD calibration of LX-17 has been conducted using the existing diameter effect data and shock shape records [3]. The new DSD fit is based off the current [2] PBX 9502 calibration and takes into account the effect of pressing density. Utilizing the PBX 9502 calibration, the effects of initial temperature can also be taken into account.

6. REFERENCES

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